National Synchrotron Programme

Singapore Synchrotron Users' Meeting 2026

10 November 2026 (Tuesday)
9.30 a.m. to 5.00 p.m.
Centre for Life Sciences, Ground Floor Auditorium

Programme and Abstracts Booklet

Table of Contents

Item	Page
Introduction to Meeting	1
National Synchrotron Programme (NSP)	2
Meeting Programme	3
Oral Paper Presentations	4 – 16
Poster Paper Presentations	17 – 31
Acknowledgements	32

© 2024 National Synchrotron Programme. All Rights Reserved.

Introduction to Meeting

The Singapore Synchrotron Users' Meeting brings together researchers and scientists from the local and regional scientific community. It creates a platform to showcase cutting-edge synchrotron-based research and investigations, providing an invaluable opportunity for knowledge exchange and collaboration. The meeting aims to keep our user community well-informed and at the forefront of the latest developments and technical advances in synchrotron science. This includes updates on the ground-breaking research carried out at the Singapore Synchrotron Light Source (SSLS) and our overseas partner facilities through the International Synchrotron Access Programme (ISAP).

This 1-day event, which serves as a gateway for both prospective and current users to explore the capabilities of the research infrastructure at SSLS and through the ISAP, where Singapore-based researchers can gain access to a comprehensive suite of state-of-the-art research facilities at our partner overseas Synchrotron facilities.

This not only expands the opportunities for collaboration but also facilitates the exchange of knowledge and expertise across borders, further enhancing the scope and impact of synchrotron-based research.

Singapore Synchrotron Users' Meeting 2026

Organised by:
National Synchrotron Programme
Supported by the National Research Foundation, Singapore

Working Committee:
Prof Mark B H Breese (Chair)
Dr Agnieszka Banas
Dr Krzysztof Banas
Ms Maryate Muhamad
Ms Christina Pang

National Synchrotron Programme (NSP)

The National Synchrotron Programme (NSP); supported by the National Research Foundation, Singapore; was officially launched on 18 October 2022.

The NSP is a national platform to promote and anchor deep capabilities in the use of Synchrotron techniques. The programme office, hosted by the National University of Singapore (NUS), brings together all Singapore-based research institutions, agencies and industry into a vibrant ecosystem of Synchrotron related research to advance knowledge, create unique tools and techniques, and develop the talent to light-up Singapore's Synchrotron efforts globally.

The Office promotes Synchrotron access through the local Singapore Synchrotron Light Source (SSLS) facility and enables access to overseas facilities through the International Synchrotron Access Programme (ISAP).

Together, these two programmes offer comprehensive access to the full range of local and international state-of-the-art beamline facilities to serve academic and industrial users across the full spectrum of physical and biomedical sciences.

Meeting Programme

Time	Paper Title / Activity	Speaker
09:00	Registration opens	
09:30	Opening and Welcome address	*Dr Krzysztof Banas SSLS, NUS*
09:40	SG-ISAP: The Past, the Present and the Future	*Prof Mark B H Breese Executive Director, NSP*
Life Sciences, Environmental Exposure & Bioimaging		
09:55	**UM26-ABS-O1** The Flaw of the Mean: High-Percentile Synchrotron XFM Reveals Temporal Shifts in Brain Heavy Metal Architecture	*Dr Agnieszka Banas SSLS, NUS*
10:15	**UM26-ABS-O11** Comparative elemental analysis of marine and freshwater Halobatinae (Heteroptera: Gerridae) with X-ray fluorescence microscopy	*Dr Chang Jia Jin Marc LKCNHM, NUS*
10:35	**UM26-ABS-O13** From Elemental Distribution to Iron Speciation: Complementary Insights from PIXE, Synchrotron XRF, and XANES	*Dr Ren Minqin CIBA/Dept of Physics, NUS*
10:55	Refreshment break, poster and networking session	
Functional Materials, Energy & Catalysis		
11:45	**UM26-ABS-O9** Electric bias-induced reversible configuration of single and heteronuclear dual-atom catalysts on 1T'-MoS_2	*Dr Wu Jianhua Dept of Chemistry, NUS*
12:05	**UM26-ABS-O10** Nanoconfined ion behavior in carbon pores: beyond partial desolvation	*Dr Wei Jiaqi School of MSE, NTU*
12:25	**UM26-ABS-O8** Hybridized Ni–O Electronic and Ni 3d Orbital Reconstruction in Samarium-Based Infinite-Layer Nickelates Revealed by X-ray Absorption Spectroscopy	*Dr Gao Xing Dept of Physics, NUS*
12:45	**UM26-ABS-O14** Synchrotron XAS of Supported Catalysts and In Situ Studies of Thermal Catalysis	*Dr Chen Xiaohan Dept of ChBE, NUS*
13:05	Lunch break, poster and networking session	
Sustainable Infrastructure & Advanced Manufacturing		
14:05	**UM26-ABS-O4** Using in situ synchrotron powder diffraction to study the hydration of Portland cement with seawater CO_2 mineralisation precipitate replacement at very early ages	*Wang Yue NUS*
14:25	**UM26-ABS-O7** Synchrotron X-ray Tomography of the Repair Interface in Underwater 3D-Printed Concrete	*Zhang Hao Dept of CEE, NUS*
14:45	**UM26-ABS-O5** Bridging length scales in metal additive manufacturing through correlative synchrotron and atom probe tomography	*Asst Prof Tan Xipeng Dept of ME, NUS*
15:05	**UM26-ABS-O12** β-solidifying α_2-based Ti-Al alloys for laser powder bed fusion: Synchrotron X-ray insight into phase retention and transformation	*Dr Ali Ghasemi Dept of ME, NUS*
15:25	Refreshment break, poster and networking session	
Structure, Function & Emerging Quantum Phenomena		
16:00	**UM26-ABS-O3** Structures that prediction cannot give: SG-ISAP-supported crystallography of enzymes and metal-binding proteins	*Dr Xue Bo SynCTI/Dept of Biochemistry, NUS*
16:20	**UM26-ABS-O6** Unravelling Hidden and Unconventional Magnetic Order with Resonant X-ray Scattering	*Dr Soh Jian Rui A*STAR*
16:40	Closing remarks and final networking session	*Dr Agnieszka Banas SSLS, NUS*
17:00	End of meeting	

UM26-ABS-O1

The Flaw of the Mean: High-Percentile Synchrotron XFM Reveals Temporal Shifts in Brain Heavy Metal Architecture

Agnieszka Banas
Singapore Synchrotron Light Source, National University of Singapore

Heavy metal accumulation in the brain is a well-established driver of neurotoxicity, yet detecting contemporary exposure routes, such as environmental particulates that act as "Trojan Horses," adsorbing and delivering concentrated metal payloads to tissue, remains analytically challenging. Standard toxicological approaches, which rely on bulk tissue analysis or mean-based statistics, tend to mask rare, high-concentration hotspots within background variation, a limitation we term "the Flaw of the Mean." To overcome this, we designed a proof-of-principle framework that pairs micrometre-resolution synchrotron X-ray Fluorescence Microscopy with robust high-percentile spatial statistics (P_{85}–P_{99}, skewness, and scale measures). Using an exploratory set of formalin-fixed paraffin-embedded human brain samples, we examined temporal changes in spatial metal distribution while distinguishing intra-tissue heterogeneity from inter-subject variation. Median concentrations showed little change over the 15-year span; however, high-percentile analysis uncovered a clear shift toward localized, tail-heavy accumulation of Nickel, Chromium, and Manganese in recent samples. Spatial correlation analysis further revealed that archival tissues showed independent trace-metal deposition, whereas contemporary samples displayed tight co-localization centered on Chromium - a pattern suggestive of a shared particulate delivery mechanism. These findings, while preliminary, show that high-percentile spatial profiling can reveal toxicological signals invisible to conventional bulk averaging.

Reference(s):

1. Nihart, A.J., Garcia, M.A., El Hayek, E. et al. Bioaccumulation of microplastics in decedent human brains. Nat Med 31, 1114–1119 (2025). https://doi.org/10.1038/s41591-024-03453-1
2. Liu, S., Wang, C., Yang, Y. et al. Microplastics in three types of human arteries detected by pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS). Journal of Hazardous Materials, Volume 469, 2024, https://doi.org/10.1016/j.jhazmat.2024.133855.
3. Dong, C. D. et al. Polystyrene microplastic particles: in vitro pulmonary toxicity assessment. *J. Hazard. Mater.* **385**, 121575 (2020); https://doi.org/10.1016/j.jhazmat.2019.121575
4. Zhu, L. et al. Tissue accumulation of microplastics and potential health risks in human. *Sci. Total Environ.* **915**, 170004 (2024). https://doi.org/10.1016/j.scitotenv.2024.170004

UM26-ABS-O3

Structures that prediction cannot give: SG-ISAP-supported crystallography of enzymes and metal-binding proteins

Xue Bo
NUS Synthetic Biology for Clinical and Technological Innovation (SynCTI) and Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore

Structure prediction has changed how we begin a project, but it has not made experiment redundant. The details we most often need, such as metal sites, ligand poses and oligomeric assemblies, are also where predicted models are least reliable. Through SG-ISAP, our group has regular access to the Australian Synchrotron for experiments that cannot be performed locally, and these beamtimes have produced most of our recent PDB entries. Four projects illustrate what this access makes possible. Ligand-bound structures of the *E. coli* glycyl radical enzymes YbiW and PflD helped establish the chemistry of anhydroglycolysis, a newly discovered metabolic pathway. Crystal structures of CL20 and CL23, lipases that synthesise bioactive FAHFA lipids, revealed C-terminus-swapped dimers and trimers where AlphaFold had predicted monomers. Structures of *Osmanthus fragrans* carotenoid cleavage dioxygenase 1 and two variants are now guiding its engineering for β-ionone production. In an EF-hand protein that binds heavy metals, anomalous scattering identified the occupied sites directly, in two crystal forms. With reliable access to beamtime, crystallography has become a routine step in our engineering cycle, and our students and postdocs gain hands-on synchrotron experience along the way.

Reference(s):

1. Terwilliger, T. C. et al. AlphaFold predictions are valuable hypotheses and accelerate but do not replace experimental structure determination. *Nat. Methods* 21, 110–116 (2024).
2. Ma, D. et al. A widespread radical-mediated glycolysis pathway. *J. Am. Chem. Soc.* 146, 26187–26197 (2024).
3. Ling, L. H. et al. Sustainable biosynthesis of diverse fatty acid esters of hydroxy fatty acids (FAHFAs) for industrial production. *ACS Sustainable Chem. Eng.* 13, 2830–2844 (2025).

UM26-ABS-O4

Using in situ synchrotron powder diffraction to study the hydration of Portland cement with seawater CO2 mineralisation precipitate replacement at very early ages

Wang Yue
National University of Singapore

Over the last decades, the cement industry has been actively pursuing decarbonization strategies, with one of the most widely adopted approaches being the partial substitution of clinker with supplementary cementitious materials [1,2]. The utilization of seawater CO_2 mineralisation precipitate (SMP), mainly composed of magnesium hydroxide and calcium carbonate [3,4], presents a promising avenue for reducing the carbon footprint of cement production. However, the early-stage hydration reactions remain less investigated, with significant data gaps critical for assessing performance.

Therefore, this study employs in situ synchrotron X-ray powder diffraction to understand the evolution of crystalline phases occurring within the first 13 hours, shedding light on the filler effect and the mechanisms behind strength development. HighScore software is used for crystal phase identification, and the diffraction data are analysed by the Rietveld method, with results compared to mass balance calculations.

The results demonstrate that replacing 10 wt% of C_3S-C_3A blend with SMP accelerates early-age C_3S hydration through a filler-induced nucleation effect, and the calcium carbonate component participates in carboaluminate reactions with C_3A to form hemicarboaluminate and monocarboaluminate. These findings demonstrate that SMP is a feasible low-carbon cement replacement and represents a promising pathway for the viability of SMP in cementitious systems.

Reference(s):

1. R. Snellings, P. Suraneni, J. Skibsted, Future and emerging supplementary cementitious materials, Cement and Concrete Research, 171 (2023).
2. S.A. Miller, V.M. John, S.A. Pacca, A. Horvath, Carbon dioxide reduction potential in the global cement industry by 2050, Cement and Concrete Research, 114 (2018) 115–124.
3. E.C. La Plante, X. Chen, S. Bustillos, A. Bouissonnie, T. Traynor, D. Jassby, L. Corsini, D.A. Simonetti, G.N. Sant, Electrolytic Seawater Mineralization and the Mass Balances That Demonstrate Carbon Dioxide Removal, ACS ES T Eng, 3 (2023) 955–968.
4. PUB, PUB partners UCLA ICM and Equatic, PUB, Singapore's National Water Agency, https://www.pub.gov.sg/Resources/News-Room/PressReleases/2024/02/PUB-partners-UCLA-ICM-and-Equatic, (2024).

UM26-ABS-O5

Bridging length scales in metal additive manufacturing through correlative synchrotron and atom probe tomography

Tan Xipeng
Department of Mechanical Engineering, College of Design and Engineering,
National University of Singapore

Metal additive manufacturing (AM) offers unprecedented design freedom but presents challenges arising from rapid solidification, non-equilibrium phase formation, chemical heterogeneity, and microstructural defects. Understanding these phenomena requires advanced characterization across multiple length scales. Here, we demonstrate a correlative approach integrating synchrotron X-ray techniques, transmission electron microscopy (TEM), and atom probe tomography (APT) to investigate microstructural evolution in additively manufactured Ni-based superalloys and NiTi shape memory alloys. Particularly, by combining APT with various in-situ synchrotron set ups, we elucidate the relationships between processing conditions, phase transformations, elemental redistribution, and properties across different material systems. This correlative framework bridges critical characterization length scales, offering deeper insights into the mechanisms governing AM processability and material performance, while highlighting the complementary capabilities of synchrotron radiation and advanced microscopy for developing high-performance additively manufactured alloys.

UM26-ABS-O6

Unravelling Hidden and Unconventional Magnetic Order with Resonant X-ray Scattering

Soh Jian Rui
Agency for Science, Technology and Research (A*STAR)

Resonant elastic X-ray scattering (REXS) is a powerful synchrotron technique for investigating complex electronic and magnetic orders in quantum materials. By exploiting element-specific resonances and polarization-dependent scattering, REXS provides microscopic insights into ordered states that are difficult to distinguish using conventional diffraction methods.

This talk presents two studies demonstrating the capabilities of resonant X-ray scattering in elucidating unconventional order in correlated materials. First, spectroscopic investigations of the double perovskite Ba2MgReO6 reveal the microscopic origin of its hidden-order phase, highlighting the interplay between spin-orbit coupling, multipolar degrees of freedom, and electronic correlations [1]. Second, REXS studies of a candidate axion insulator EuIn2As2 uncover the nature of its unconventional magnetic order, demonstrating how resonant scattering can identify magnetic structures relevant to emergent topological phenomena [2].

Together, these studies illustrate how synchrotron-based resonant X-ray techniques can resolve subtle electronic and magnetic ordering phenomena and establish connections between microscopic order parameters and macroscopic quantum properties. The results highlight the importance of element-specific spectroscopic probes in advancing our understanding of complex quantum materials and demonstrate the broader potential of synchrotron science for exploring emergent states of matter.

Reference(s):

1. *Spectroscopic signatures and origin of hidden order in Ba2MgReO6,* Jian-Rui Soh, Maximilian E. Merkel, Leonid V. Pourovskii, Ivica Živković, Oleg Malanyuk, Jana Pásztorová, Sonia Francoual, Daigorou Hirai, Andrea Urru, Davor Tolj, Dario Fiore Mosca, Oleg V. Yazyev, Nicola A. Spaldin, Claude Ederer & Henrik M. Rønnow, **Nature Communications 15**, 10383 (2024).
2. *Understanding unconventional magnetic order in a candidate axion insulator by resonant elastic x-ray scattering* Jian-Rui Soh, Alessandro Bombardi, Frédéric Mila, Marein C. Rahn, Dharmalingam Prabhakaran, Sonia Francoual, Henrik M. Rønnow & Andrew T. Boothroyd **Nature Communications 14**, 3387 (2023).

UM26-ABS-O7

Synchrotron X-ray Tomography of the Repair Interface in Underwater 3D-Printed Concrete

Zhang Hao
Department of Civil and Environmental Engineering, College of Design and Engineering, National University of Singapore

Underwater three-dimensional concrete printing (U3DCP) offers a promising approach for repairing submerged concrete structures. However, the integrity of the interface between existing concrete substrates and printed repair materials remains a critical concern, particularly due to potential water entrapment and internal defects.

This study employs synchrotron X-ray computed tomography (CT) to investigate the internal structure of underwater-printed concrete repairs. Cylindrical specimens were extracted from repaired elements, with CT imaging focused on a region approximately 20–30 mm above and below the repair interface. Preliminary CT reconstructions reveal heterogeneous internal features, including potential voids, while post-compression observations show visible cracking. These initial observations provide a basis for further investigation of possible relationships between internal defects and mechanical failure.

Ongoing work will quantify pore size, spatial distribution, and connectivity, and examine the effects of freshwater and seawater environments. The findings aim to improve understanding of interfacial integrity and support the assessment of underwater 3D-printed concrete repair performance.

UM26-ABS-O8

Hybridized Ni–O Electronic and Ni 3d Orbital Reconstruction in Samarium-Based Infinite-Layer Nickelates Revealed by X-ray Absorption Spectroscopy

Gao Xing
Department of Physics, Faculty of Science, National University of Singapore

Understanding the electronic structure of infinite-layer nickelates is crucial for elucidating the mechanism of superconductivity in this emerging family of unconventional superconductors. In particular, the interplay among Ni 3*d* orbitals, O 2*p* ligand states, and rare-earth ions remains unresolved. Here, we investigate superconducting Eu-doped infinite-layer $Sm_{1-x-y}Eu_xCa_yNiO_2$ thin films using multi-edge X-ray absorption spectroscopy together with temperature-dependent X-ray linear dichroism. Topotactic reduction from the perovskite precursor to the infinite-layer phase produces a substantial electronic reconstruction, including a reduced Ni valence, a suppression of ligand-hole spectral weight, and a pronounced increase of Eu^{2+} fraction. While Eu doping produces only subtle changes in the average Ni valence, but strongly modifies the hybridized Ni-O electronic states. The O *K*-edge pre-edge weight and Ni L_3 peak intensity track the superconducting dome, indicating that optimized Ni-O hybridization is closely associated with superconductivity. Temperature-dependent XLD shows a sign reversal of the dichroic response upon cooling in the superconducting compositions, supporting a multiorbital electronic structure and indicating a temperature-dependent orbital reconstruction between $3d_{x2-y2}$ and $3d_{3z2-r2}$. These results establish doping- and temperature-dependent reconstruction of hybridized Ni–O states as a key spectroscopic feature of superconducting infinite-layer nickelates.

Reference(s):

1. Chow, S. L. E., Luo, Z. & Ariando, A. Bulk superconductivity near 40 K in hole-doped SmNiO2 at ambient pressure. *Nature* **642**, 58–63 (2025).
2. Zeng, S. *et al.* Origin of a Topotactic Reduction Effect for Superconductivity in Infinite-Layer Nickelates. *Phys. Rev. Lett.* **133**, 066503 (2024).
3. Zeng, S. W. *et al.* Observation of perfect diamagnetism and interfacial effect on the electronic structures in infinite layer Nd0.8Sr0.2NiO2 superconductors. *Nat. Commun.* **13**, 743 (2022).
4. Rubi, K. *et al.* High-field-stabilized reentrant superconductivity in infinite-layer nickelate thin films. *Nat. Commun.* https://doi.org/10.1038/s41467-026-75922-9 (2026) doi:10.1038/s41467-026-75922-9.

UM26-ABS-O9

Electric bias-induced reversible configuration of single and heteronuclear dual-atom catalysts on 1T'-MoS2

Wu Jianhua
Department of Chemistry, Faculty of Science, National University of Singapore

The development of substrates capable of anchoring single-atom catalysts (SACs) while enabling their dynamic reconfiguration into heteronuclear dual-atom catalysts (DACs) holds considerable promise for electrochemical synthesis, yet remains underexplored. Here we show that electrochemical desulfurization of MoS2 generates vacancy-rich 1T′ domains, which support high loadings of Cu (7.9 wt%) and Pt (6.7 wt%) SACs that are well-positioned for dynamic sintering to form DACs. Operando X-ray absorption spectroscopy and density functional theory calculations reveal a voltage-driven, reversible transformation between individual Pt/Cu SACs and Cu–Pt DAC configurations during hydrogen evolution reaction potentials. The electric-field-induced Cu–Pt DACs exhibit superior performance in the selective hydrogenation of alkynes compared with their monometallic SAC counterparts. This work underscores vacancy-enriched 1T′-MoS2 as a versatile platform for high-density SAC deposition, enabling on-demand structural reconfiguration and paving the way for tailored catalyst design in electrosynthesis.

Reference(s):

1. Wu, J., Chen, Z., Yang, K. *et al.* Electric bias-induced reversible configuration of single and heteronuclear dual-atom catalysts on 1T'-MoS2. *Nat. Nanotechnol.* **20**, 1043–1051 (2025). https://doi-org.libproxy1.nus.edu.sg/10.1038/s41565-025-01934-z

UM26-ABS-O10

Nanoconfined ion behavior in carbon pores: beyond partial desolvation

Wei Jiaqi
School of Materials Science & Engineering, Nanyang Technological University

Ion behavior under nanoconfinement governs a wide range of electrochemical processes. However, it remains difficult to directly resolve how solvated ions reorganize, interact, and migrate inside electrified nanopores, as the solvation geometry, ion-ion association, and pore accessibility become strongly coupled. Herein, we recently use synchrotron X-ray absorption spectroscopy (XAS) to reveal two distinct but connected forms of nanoconfined ion reorganization in carbon electrodes.

First, we observed metal-ion oligomerization inside electrified carbon micropores. This confined complexation process alters the local ionic structure and provides a mechanistic explanation for activation behavior, capacity loss, and recoverable “buried” charge storage in aqueous capacitive systems. Second, we extended this framework to multivalent metal ions with well-defined solvation shells, showing that nanopores can induce solvation-shell folding rather than simple desolvation. By combining quantitative XAS with pore-size-resolved physical modelling, we establish how the confinement-dependent solvation geometry controls ion adsorption, accessible pore volume, and rate capability across different metal ions and carbon pore structures.

Together, these studies suggest that nanoconfined ions should be treated as adaptive coordination entities whose structure evolves with pore size, potential, and local packing. More broadly, synchrotron XAS offers a powerful route to connect local ion structure with macroscopic charge-storage behavior in liquid electrochemical environments.

Reference(s):

1. **Wei, J.**; Zhong, L.; Xi, S.; Salanne, M.; Chen, X.; Li, S.; et al. Metal-Ion Oligomerization Inside Electrified Carbon Micropores and its Effect on Capacitive Charge Storage. *Adv. Mater.* **2022**, *34*, 2107439.
2. **Wei, J.**; Xi, S; Iadecola A.; Diao, C.; Johannessen, B.; Chen, X.; Salanne, M.; Li, S.; Protocols on X-ray Absorption Spectroscopy Measurement and Interpretation. *ACS Nano*, **2026**, *20*, 25226

UM26-ABS-O11

Comparative elemental analysis of marine and freshwater Halobatinae (Heteroptera: Gerridae) with X-ray fluorescence microscopy

Chang Jia Jin Marc
Lee Kong Chian Natural History Museum, National University of Singapore

Water-skaters of the genus *Halobates* (Heteroptera: Gerridae) are unique among insects, with five species that have adapted to a completely oceanic lifestyle. While their superhydrophobic properties are well-studied, little is known about how they cope with other environmental stressors in the open ocean. Here, we employed synchrotron X-ray fluorescence microscopy (SXFM), a technique enabling multidimensional visualization of millimetre-sized, non-translucent specimens, to investigate whether elemental composition and distribution contribute to open-ocean adaptation. We imaged the oceanic *Halobates micans* and coastal *Halobates hayanus*, and compared them with freshwater relatives *Ventidius harrisoni* and *Metrocoris tenuicornis*. Across elements ranging from sulphur to strontium (atomic numbers 16–38), only minor differences were detected, which likely reflected preservation methods rather than habitat-specific adaptations. SXFM effectively revealed elemental distributions across insect bodies, highlighting its potential for detecting heavy metals and resolving physiological processes at fine scales. We hypothesize that elevated concentrations and specific spatial distributions of elements such as Mn, Fe, Cu, Zn, and Se in *Halobates* may enhance resilience to UV-induced cellular damage, thereby contributing to survival in extreme marine environments. This work provides a foundation for future studies into the adaptive strategies of water-skaters and opens avenues for bio-inspired applications in materials science and technology.

Reference(s):

1. G.A. Mahadik, J. F. Hernandez-Sanchez, S. Arunachalam, et al. 2020 Superhydrophobicity and size reduction enabled *Halobates* (Insecta: Heteroptera, Gerridae) to colonize the open ocean. *Scientific Reports*, 10: 7785.
2. L. Cheng. 1973. Marine and freshwater skaters: differences in surface fine structures. *Nature*, 242(5393): 132–133.
3. L. Cheng. 1985. Biology of *Halobates* (Heteroptera: Gerridae). *Annual Review of Entomology*, 30: 111135.
4. L. Cheng, M. Douek and D.A.I. Goring. 1978. UV absorption by gerrid cuticles. *Limnology and Oceanography*, 23(3): 554–556.

UM26-ABS-O12

β-solidifying α_2-based Ti-Al alloys for laser powder bed fusion: Synchrotron X-ray insight into phase retention and transformation

Ali Ghasemi
Department of Mechanical Engineering, College of Design and Engineering,
National University of Singapore

Historically brittle α_2-Ti_3Al alloys are difficult to process. High-energy synchrotron X-ray diffraction (SXRD) was used to reveal how a deliberately β-solidifying alloy, Ti-28Al-2.4Nb-0.6Mo-1.8V (at%), retains a crack-tolerant phase during laser powder bed fusion and transforms into a service-relevant α/α_2 microstructure on heating. The alloy was produced by in-situ alloying 60 wt% TNM-B1 and 40 wt% Ti-6Al-4V powders, yielding crack-free parts with approximately 99.9% relative density. Room-temperature SXRD showed that the as-built microstructure was dominated by metastable β with weak B2 ordering (B2{100}/β{110} intensity ratio approximately 0.05). In-situ high-temperature SXRD from 300 to 600 °C resolved a staged sequence comprising partially ordered β/B2, disordered β, disordered α, and partially ordered α/α_2, with α_2 superlattice reflections emerging above approximately 500 °C. Guided by these observations, a post-build heat treatment at 600 °C for 8 h eliminated β/B2 and generated an α/α_2-dominated structure. The treated alloy achieved 356.9 MPa ultimate tensile strength and 4.7% total strain at 750 °C. These results demonstrate how synchrotron diffraction can directly guide alloy design and thermal processing for additively manufactured titanium aluminides.

Reference(s):

1. H. A. Soliman, A. Ghasemi, M. Elbestawi, T. Okajima, and S. L. Sing, “β-solidifying α_2-based Ti-Al alloys for laser powder bed fusion: Synchrotron X-ray insight into phase retention and transformation,” Journal of Alloys and Compounds, vol. 1069, 188592, 2026. https://doi.org/10.1016/j.jallcom.2026.188592

UM26-ABS-O13

From Elemental Distribution to Iron Speciation: Complementary Insights from PIXE, Synchrotron XRF, and XANES

Ren Minqin
Centre for Ion Beam Applications, Department of Physics, Faculty of Science,
National University of Singapore

Understanding the elemental distribution and chemical speciation of iron in biological tissues is essential for investigating its role in physiological & pathological processes. This work compares two approaches to elemental analysis of thin biological tissue sections: laboratory-based Proton-Induced X-ray Emission (PIXE) & synchrotron-based X-ray Fluorescence Analysis (XRF). Both techniques enable multi-elemental mapping of biologically relevant elements, including Fe, P, S, K, Ca, Cu, and Zn, but differ in their analytical capabilities, instrumental requirements, & accessibility.

The presentation focuses on comparing the advantages and limitations of both methods, particularly regarding spatial resolution, detection sensitivity, quantitative capabilities, acquisition time, and sample preparation requirements.

Additionally, given the crucial role of iron oxidation states in biological processes, Fe K-edge X-ray Absorption Near-Edge Structure (XANES) spectroscopy was employed at the synchrotron facility to investigate iron speciation, particularly the distinction between Fe^{2+} and Fe^{3+}.

Our study highlights the benefits and limitations of laboratory-based & synchrotron-based techniques, demonstrating how their complementary capabilities can provide a more comprehensive understanding of elemental distributions and iron chemistry in biological tissues.

Reference(s):

1. Iron and atherosclerosis: Lessons learned from rabbits relevant to human disease, Barry Halliwell, Frank Watt and Ren Minqin, Free Radical Biology and Medicine, 209, P165-170, 2023
2. Quantitative analysis of multiple elements in healthy and remodeled epithelium from human upper airway mucosa using nuclear microscopy, M.-Q. Ren, Y.-T. Zhou, H.-X. Chen, T.-Y. Li, S. K. Vajandar, T. Osipowicz, F. Watt, C.-W. Li, Allergy Vol 73, issue 3, P724-727, 2018
3. Analytical possibilities of highly focused ion beams in biomedical field, M.Q. Ren, X Ji, S.K. Vajandar, Z.H. Mi, A. Hoi, T Walczyk, J.A. van Kan, A.A. Bettiol, F. Watt, T. Osipowicz, Nuclear Instrument and Methods in Physics Research B Vol 406, P15-24, 2017
4. Does iron inhibit calcification during atherosclerosis? Reshmi Rajendran; Ren Minqin; John A Ronald; Brian K Rutt; Barry Halliwell; Frank Watt; Free Radical Biology and Medicine, Vol. 53(9), P1675-1679, 2012
5. Distribution and chemical state analysis of iron in the Parkinsonian substantia nigra using synchrotron radiation micro beams, Ari Ide-Ektessabi, Takuo Kawakami and Frank Watt, NIMB Vol.213, P590–594, 2004
6. Correlation of iron and zinc levels with lesion depth in newly formed atherosclerotic lesions, Ren Minqin, Frank Watt, Benny Tan Kwong Huat and Barry Halliwell, Free Radical Biology and Medicine, Vol.34(6), P746-752, 2003

UM26-ABS-O14

Synchrotron XAS of Supported Catalysts and In Situ Studies of Thermal Catalysis

Chen Xiaohan
Department of Chemical and Biomolecular Engineering, College of Design and Engineering, National University of Singapore

Supported metal catalysts can undergo changes in oxidation state and local coordination during activation and reaction, complicating the identification of catalytically relevant structures. This presentation highlights our X-ray absorption spectroscopy (XAS) studies at the Synchrotron Light Research Institute (SLRI), Thailand, and explores in situ experimental approaches for thermal catalysis. X-ray absorption near-edge structure and extended X-ray absorption fine structure analyses are used to examine metal oxidation states, metal–oxygen and metal–metal coordination, and the effects of support composition. Particular attention is given to linking these structural characteristics with catalyst reducibility, dispersion and metal–support interactions through complementary characterisation. Building on these studies, we discuss in situ XAS experiments combining controlled heating and gas switching to investigate catalyst evolution during reduction and thermal reactions, with CO_2 hydrogenation and methane conversion as representative applications. Experimental considerations include sample preparation, reaction-cell configuration, gas delivery, temperature control and spectral acquisition. Correlating structural evolution with catalytic performance provides a basis for understanding catalyst activation and stability. This work highlights the value of SLRI access for advancing in situ methodologies and the structural understanding of supported catalysts.

UM26-ABS-P1

Falcilysin: a common target of antimalarial compounds

Lin Jianqing
NTU Institute of Structural Biology, Nanyang Technological University

Malaria is a widespread infectious disease in tropical and subtropical regions, causing approximately half a million deaths worldwide each year. The emergence of drug-resistant parasites has reduced the efficacy of existing antimalarial drugs, highlighting the need for new therapeutic targets and compounds.

Falcilysin, an M16C zinc metallopeptidase involved in the hemoglobin degradation pathway, is essential for Plasmodium falciparum survival and represents an attractive antimalarial drug target. Mass spectrometry-based cellular thermal shift assay (MS-CETSA) identified falcilysin as a potential target of several antimalarial compounds, including chloroquine, mefloquine, MK-4815, MMV000848, and MMV665806. However, MS-CETSA alone does not establish direct protein–compound interactions, necessitating experimental validation.

In this study, we combined biochemical and biophysical approaches with X-ray crystallography and cryo-EM to validate these interactions and elucidate the molecular mechanism of falcilysin inhibition. X-ray crystallography revealed a common compound-binding pocket distinct from the active site, providing structural evidence for an allosteric mode of inhibition. Cryo-EM further revealed compound-induced conformational changes associated with inhibition of falcilysin activity, providing mechanistic insights into its potential as a drug target.

Reference(s):

1. Wirjanata G, Lin J, Dziekan JM, El Sahili A, Chung Z, Tjia S, Binte Zulkifli NE, Boentoro J, Tham R, Jia LS, Go KD, Yu H, Partridge A, Olsen D, Prabhu N, Sobota RM, Nordlund P, Lescar J, Bozdech Z. Identification of an inhibitory pocket in falcilysin provides a new avenue for malaria drug development. Cell Chem Biol. 2024 Apr 18;31(4):743-759.e8. doi: 10.1016/j.chembiol.2024.03.002. Epub 2024 Apr 8. PMID: 38593807.
2. Lin J, Yan X, Chung Z, Liew CW, El Sahili A, Pechnikova EV, Preiser PR, Bozdech Z, Gao YG, Lescar J. Inhibition of falcilysin from Plasmodium falciparum by interference with its closed-to-open dynamic transition. Commun Biol. 2024 Aug 31;7(1):1070. doi: 10.1038/s42003-024-06774-6. PMID: 39217277; PMCID: PMC11365994.

UM26-ABS-P2

Soft X-ray Spectroscopy at the SINS Beamline, Singapore Synchrotron Light Source: Capabilities and Recent Scientific Highlights

Yu Xiaojiang
Singapore Synchrotron Light Source, National University of Singapore

The Surface, Interface and Nanostructure Science (SINS) beamline at the Singapore Synchrotron Light Source (SSLS) provides versatile soft X-ray spectroscopy capabilities for investigating the chemical, electronic and magnetic properties of functional materials. Operating over 40–1200 eV with selectable linear and circular polarization, the beamline supports X-ray photoelectron spectroscopy (XPS), angle-resolved photoemission spectroscopy (ARPES), X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD).

This presentation highlights three recent user studies demonstrating the scientific impact of complementary XPS and near-edge X-ray absorption fine structure (NEXAFS) measurements at SINS. In UV-treated nickel–iron Prussian blue analogue electrocatalysts, XPS and transition-metal L-edge NEXAFS revealed the formation of oxide/oxyhydroxide species associated with enhanced oxygen evolution activity [1]. In ionic-ZIF-8-derived nickel single-atom catalysts, complementary spectroscopic measurements elucidated the Ni–N_4 coordination environment and elongated Ni–N bonding associated with improved CO selectivity during electrochemical CO_2 reduction [2]. In crystalline graphitic carbon nitride photocatalysts, C and N K-edge NEXAFS and XPS revealed changes in chemical bonding and nitrogen coordination associated with enhanced photocatalytic hydrogen evolution [3].

These studies demonstrate the scope of SINS in elucidating electronic structure and structure–property relationships, supporting synchrotron users' research in catalysis, energy conversion and advanced functional materials.

Reference(s):
1. R. S. U. Haq et al., *Chemical Engineering Journal* 523, 168369 (2025).
2. M. Sun et al., *Advanced Functional Materials* (2025).
3. X. Chu et al., *Electron* (2025).

UM26-ABS-P3

Rationally Designed Flexible Covalent Organic Frameworks for the Efficient Separation

Ji Chunqing
Department of Chemical and Biomolecular Engineering, College of Design and Engineering, National University of Singapore

The separation and purification of light hydrocarbons (LHs) are critical yet energy-intensive processes in the chemical industry. Adsorptive separation using porous materials offers a promising energy-efficient alternative to conventional technologies. Among emerging porous materials, covalent organic frameworks (COFs) have attracted considerable attention owing to their well-defined structures, tunable pore environments, and excellent chemical stability. In particular, framework flexibility, including breathing and gate-opening behaviors, provides unique opportunities for selective molecular recognition and separation. Herein, we report the rational design and synthesis of NUS-700, an iptycene-based, non-interpenetrated flexible COF featuring a dynamically adaptable framework. Gas adsorption measurements reveal distinctive adsorption behaviors toward light hydrocarbons, including C_2H_2, C_2H_4, and C_2H_6, at 195 K, suggesting guest-responsive structural transformations. These dynamic structural responses are further investigated using in situ powder X-ray diffraction (PXRD) coupled with gas adsorption measurements, enabling direct monitoring of framework evolution during gas uptake. Furthermore, synchrotron PXRD measurements under activated and liquid-phase conditions provide additional evidence of framework flexibility and structural rearrangements in response to different environments. Collectively, these investigations establish correlations between framework dynamics, host–guest interactions, and selective adsorption behavior, offering valuable insights into the rational design of flexible COFs for energy-efficient hydrocarbon separation.

UM26-ABS-P4

Synchrotron-Enabled Phase Characterization of Nickel-Free High-Nitrogen Stainless Steels for Advanced Engineering Applications

Chew Li Tian
Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR)

Nickel-free high-nitrogen stainless steels offer a promising alternative to conventional stainless steels by reducing nickel dependency while providing desirable mechanical and corrosion properties. However, maintaining austenite stability and suppressing undesirable secondary phase formation remain key challenges during alloy processing.

This study investigates additively manufactured nickel-free nitrogen-alloyed stainless steels using synchrotron X-ray diffraction (XRD) and Rietveld refinement to identify and quantify crystalline phases, with particular emphasis on austenite stability and potential nitride or carbide precipitation.

Synchrotron XRD revealed predominantly austenitic microstructures, with no detectable crystalline nitrides or carbides within the measurement limits. These findings are consistent with nitrogen retention in solid-solution, suggesting its contribution to austenite stabilization and strengthening. The developed alloys achieved majority austenite, relative densities exceeding 99.5%, and ultimate tensile strengths above 900 MPa. Corrosion performance was also evaluated, although the contribution of interstitial nitrogen requires further investigation.

These findings demonstrate the value of SG-ISAP-supported synchrotron characterization in advancing the understanding and development of nickel-free nitrogen-alloyed steels, highlighting their potential for further development in medical, nuclear, and marine engineering applications.

Reference(s):

1. Baisong Cheng, et al., (2022) Ambient pressure fabrication of Ni-free high nitrogen austenitic stainless steel using laser powder bed fusion method, Additive Manufacturing, 55, 102810
2. Teh, W.H., et al. (2026). Low-temperature Fe–N enabled austenite stabilization in nickel-free nitrogen-alloyed stainless steels. Materials & Design, 264, 115719.

UM26-ABS-P5

Nickel Geminal-Atom Catalysts for Cross-Coupling Reactions: Synchrotron-Based Structural Insights

Cai Qilong
Department of Chemistry, Faculty of Science, National University of Singapore

Heterogeneous single-atom catalysts (SACs) offer well-defined active sites but often suffer from rigid coordination environments that hinder cooperative substrate activation. To overcome this limitation, we previously developed copper-based geminal-atom catalysts (Cu-GACs), featuring neighbouring low-valent Cu centres anchored on polymeric carbon nitride (PCN). Their dynamic coordination environments enable cooperative activation of multiple substrates, facilitating diverse C–X (X = C, N, O, S) cross-coupling reactions.

Building on this concept, we further extended the GAC platform to nickel (Ni-GACs) to address more challenging carbon–carbon bond-forming transformations. Synchrotron-based X-ray absorption spectroscopy (XAS) provides insights into the electronic structures and local coordination environments of the metal centres, supporting the structural characterisation of GACs. Catalytic investigations demonstrate efficient C(sp^2)–C(sp^2) Suzuki coupling involving aryl chlorides and bromides, alongside promising reactivity in C(sp^2)–C(sp^3) coupling reactions. Moreover, Ni-GACs can be synthesised on a scale exceeding 10 g while maintaining good recyclability and stability.

These findings demonstrate the versatility and scalability of GACs and highlight the importance of synchrotron-based characterisation in guiding the development of cooperative heterogeneous catalysts for challenging organic transformations.

Reference(s):
1. Hai, X. et al. Geminal-atom catalysis for cross-coupling. *Nature* **622**, 754–760 (2023).
2. Hai, X. et al. Scalable two-step annealing method for preparing ultra-high-density single-atom catalyst libraries. *Nat. Nanotechnol.* **17**, 174–181 (2022).
3. Wang, Q. et al. Geminal atom catalysts with minimized d-orbital holes enable β-elimination-resistant C(sp^2)–C(sp^3) cross-coupling. *J. Am. Chem. Soc.* **148**, 16138–16150 (2026).

UM26-ABS-P6

Unravelling Metal–Support Interactions and Their Effects on Catalytic Performance through Synchrotron-Based X-ray Absorption Spectroscopy

Cao Yuan
Department of Chemical and Biomolecular Engineering, College of Design and Engineering, National University of Singapore

Metal–support interactions and size effects play crucial roles in regulating the electronic structures and catalytic performance of electrocatalysts [1,2,3]. Here, carbon-supported nickel (Ni) catalysts, ranging from single atoms and clusters to nanoparticles, are employed as model systems to systematically investigate the influence of metal size and metal–support interactions on electrocatalytic performance. Synchrotron-based X-ray absorption spectroscopy (XAS) is employed to investigate the electronic structures, oxidation states, and local coordination environments of Ni species with different sizes [3], with particular emphasis on how size variations affect interfacial charge transfer and electronic interactions between Ni and carbon supports. By correlating the spectroscopic findings with electrocatalytic performance, this study aims to elucidate the interplay between size effects and metal–support interactions and establish fundamental structure–activity relationships, providing valuable guidance for the rational design of efficient Ni-based electrocatalysts for sustainable energy conversion.

Reference(s):

1. Shi, X.; Wen, Z.; Gu, Q.; et al. Metal–support frontier orbital interactions in single-atom catalysis. Nature 2025, 640, 668–675.
2. Liu, L.; Corma, A. Metal Catalysts for Heterogeneous Catalysis: From Single Atoms to Nanoclusters and Nanoparticles. Chem. Rev. 2018, 118 (10), 4981–5079.
3. Gloag, L.; Somerville, S. V.; Gooding, J. J.; Tilley, R. D. Co-catalytic Metal–Support Interactions in Single-Atom Electrocatalysts. Nat. Rev. Mater. 2024, 9, 173–189.
4. Microenvironment reconstitution of highly active Ni single atoms on oxygen-incorporated Mo_2C for water splitting. Nat. Commun. 2024, 15, 1342.

UM26-ABS-P7

Investigating the Operando Dynamic Evolution of Geminal-Atom Nanozymes for Hydrolytic Reaction Involving Multiple Intermediates Using XAFS

Li Jun
Department of Chemistry, Faculty of Science, National University of Singapore

Hydrolytic reactions catalysed by bimetalloenzymes play a vital role in biological systems and industrial processes [1,2], yet their mechanisms typically involve multiple reaction intermediates and dynamic active-site rearrangements [3]. This complexity makes it challenging to rationally design highly active single-atom nanozymes that mimic bimetalloenzyme hydrolysis, and it also hampers mechanistic investigation at the atomic level [4]. In this work, we propose and develop a class of geminal-atom nanozymes (GAzymes) incorporating paired metal centers (Mn, Fe, Co, Ni, Cu, and Zn) in close spatial proximity to emulate bimetallic enzymatic active sites. These GAzymes exhibit efficient hydrolytic activity across representative reactions, demonstrating their ability to replicate key functional features of natural bimetalloenzymes. Preliminary experimental results further reveal that the two dynamic metal sites in GAzymes display pronounced selectivity toward hydrolytic substrates. We therefore hypothesize that GAzymes enable dynamic co-adsorption of water molecules and substrates on dual metal centers, stabilizing low-energy reaction intermediates and thereby lowering the energy barrier for bond cleavage during hydrolysis. This study provides valuable insights into atomically precise hydrolytic catalysis and offers a promising framework for the rational design of next-generation nanozymes and mechanistic understanding of hydrolytic reactions.

Reference(s):

1. S. Mondal, P. Myers, S. Zhang. Unsymmetric bimetallic centres in metalloproteins and synthetic models. ***Nat. Rev. Chem.*** 2025, doi.org/10.1038/s41570-025-00781-9.
2. Z. Zhang, Z. Chen, Y. Zhang, et al. Leveraging mechanistic insight to design hydrolytic nanozymes. ***Coord. Chem. Rev.*** 2025, 524, 216340.
3. J. Brem, T. Panduwawala, J. U. Hansen, et al. Imitation of β-lactam binding enables broad-spectrum metallo-β-lactamase inhibitors. ***Nat. Chem.*** 2022, 14, 15–24.
4. X. Hai, Y. Zheng, Q. Yu, et al. Geminal-atom catalysis for cross-coupling. ***Nature*** 2023, 622, 754–760.

UM26-ABS-P8

Investigating Cu partitioning and its antibacterial response for 4D-printed NiTiCu

Guo Jinxi
Department of Mechanical Engineering, College of Design and Engineering,
National University of Singapore

Heat treatment intended to homogenise additively manufactured NiTiCu produces a non-linear antibacterial response. Understanding this behaviour requires resolving Cu partitioning. NiTiCu fabricated by laser powder bed fusion with in-situ alloying exhibits its strongest antibacterial activity in the as-built condition. Activity decreases markedly after 1 h at 820 °C and partially recovers with longer treatment, remaining below the as-built level after 10 h. We hypothesise that Cu redistribution, involving dissolution and subsequent precipitation, contributes to this evolution. Synchrotron small-angle X-ray scattering (SAXS) reveals global scattering differences between selected as-built and 10 h heat-treated regions. Transmission electron microscopy shows particles spanning different sizes in both conditions, while atom probe tomography (APT) maps the exact chemistry of local Cu enrichment. Correlative analysis will verify microstructural interpretations with both local chemistry and global scattering [1]. We propose using APT-derived composition and spatial correlations to constrain forward SAXS calculations and extract interpretable microstructural descriptors. Linked to processing histories and measured properties, these descriptors could train uncertainty-aware models to prioritise alloy compositions and heat treatments for experimental validation [2]. This NiTiCu study provides a test case for integrating local chemical information and synchrotron scattering towards data-informed alloy design.

Reference(s):

1. A. Biswas et al., Acta Materialia 116 (2016) 219-230. https://doi.org/10.1016/j.actamat.2016.06.043
2. D. Khatamsaz et al., npj Computational Materials 9 (2023) 221. https://doi.org/10.1038/s41524-023-01173-7

UM26-ABS-P9

Data-Driven Discovery of Salt-Solvent-Solvation Interplay Governing Optimal Precycling Temperature for High-Rate Lithium-Ions Batteries

Tan Fu Lun
Nanyang Technological University

Electrolyte engineering for high-rate lithium-ion batteries (LIBs) has predominantly focused on molecular composition, often overlooking the critical role of temperature during battery formation (BF). Here, we establish precycling temperature (PT) as a tunable parameter for engineering cathode–electrolyte interphase (CEI) properties and enhancing rate capability. By systematically investigating lithium difluoro(oxalato)borate (LiDFOB)-based ether electrolytes with varying ether solvents and PTs, we reveal a salt–solvent–solvation interplay governing the temperature-dependent electrochemical response. Electrochemical rate tests and impedance spectroscopy demonstrate that lower-temperature formation generally improves high-rate capability, whereas elevated formation temperatures increase interfacial resistance. Variable-temperature nuclear magnetic resonance (NMR) and synchronous small- and wide-angle X-ray scattering (SWAXS) elucidate temperature-dependent solvation reconfiguration, while surface-sensitive spectroscopies reveal corresponding changes in CEI composition. Notably, increased LiF formation under lower-temperature conditions does not simply correlate with increased contact ion pairs or aggregates, challenging conventional assumptions that greater anion participation necessarily promotes beneficial interphase chemistry. Instead, these findings suggest that the relationship between solvation structure, interphase evolution, and lithium-ion transport is strongly dependent on the coupled salt–solvent environment and formation kinetics. This work establishes a mechanistic framework for understanding PT as an electrolyte-specific design variable toward rational optimization of BF protocols for fast charging LIBs.

Reference(s):

1. Wood, D. L., III; Li, J.; An, S. J. Formation Challenges of Lithium-Ion Battery Manufacturing. *Joule* **2019**, *3*, 2884-2888.
2. Lei, S.; Zeng, Z.; Cheng, S.; Xie, J. Fast-charging of lithium-ion batteries: A review of electrolyte design aspects. *Battery Energy* **2023**, *2*, 20230018.
3. Hong, L.; Zhang, Y.; Mei, P.; Ai, B.; Zhang, Y.; Zhou, C.; Bao, X.; Zhang, W. Temperature-Responsive Formation Cycling Enabling LiF-Rich Cathode-Electrolyte Interphase. *Angew. Chem. Int. Ed.* **2024**, *63*, e202409069.
4. Mo, Y.; Liu, G.; Chen, J.; Zhu, X.; Peng, Y.; Wang, Y.; Wang, C.; Dong, X.; Xia, Y. Unraveling the temperature-responsive solvation structure and interfacial chemistry for graphite anodes. *Energy Environ. Sci.* **2024**, *17*, 227-237, 10.1039/D3EE03176D.
5. Zhu, Z.; Cao, S.; Ge, X.; Xi, S.; Xia, H.; Zhang, W.; Lv, Z.; Wei, J.; Chen, X. Enabling the High-Voltage Operation of Layered Ternary Oxide Cathodes via Thermally Tailored Interphase. *Small Methods* **2022**, *6*, 2100920.
6. Yuan, S.; Cao, S.; Chen, X.; Wei, J.; Lv, Z.; Xia, H.; Chen, L.; Ng, R. B. F.; Tan, F. L.; Li, H.; et al. Anion-Modulated Solvation Sheath and Electric Double Layer Enabling Lithium-Ion Storage From −60 to 80 °C. *J. Am. Chem. Soc.* **2025**, *147*, 4089-4099.

UM26-ABS-P10

Deciduous Teeth as a Window into Early-Life Respiratory Health: Pilot Synchrotron Evidence

Huang Yongmao
Faculty of Dentistry, National University of Singapore

Objectives: Respiratory illness in infancy is common, but its systemic impact is hard to assess retrospectively. Deciduous teeth grow from before birth into infancy and record early-life chemistry. We asked whether infant respiratory illness leaves an elemental signature.

Methods: Lower central deciduous incisors from 10 children with neonatal respiratory morbidity and 44 controls (GUSTO cohort, Singapore) were mapped for Ca, Zn and Sr by synchrotron X-ray fluorescence microscopy at 1–2 μm. The neonatal line, located by polarised-light microscopy, placed each map on a timeline around birth. Groups were compared by permutation tests with false-discovery-rate control.

Results: Zn was higher in case teeth in all 30 comparisons of Zn level or Zn/Ca. Dentine Zn was 22% higher in cases (Cliff's delta 0.60, q = 0.07), one of three of 86 measurements passing correction. Zn/Ca was already higher before birth (enamel, last three months: +52%, Holm-adjusted p = 0.016) and remained higher without a change at birth, also after adjustment for section thickness.

Conclusions: Teeth of children with neonatal respiratory morbidity carry more Zn, already before birth. Linking it with each child's illness history, gestational age and feeding will test whether it marks infant respiratory illness.

Reference(s):

1. Dean MC, Spiers KM, Garrevoet J, Le Cabec A. Synchrotron X-ray fluorescence mapping of Ca, Sr and Zn at the neonatal line in human deciduous teeth reflects changing perinatal physiology. Arch Oral Biol 2019;104:90–102. https://doi.org/10.1016/j.archoralbio.2019.05.024.
2. Howard DL, de Jonge MD, Afshar N, Ryan CG, Kirkham R, Reinhardt J, et al. The XFM beamline at the Australian Synchrotron. J Synchrotron Radiat 2020;27(5):1447–58. https://doi.org/10.1107/S1600577520010152.

UM26-ABS-P11

Birth-anchored synchrotron XFM of deciduous teeth from children with atopic dermatitis: a pilot window into prenatal and early-postnatal development

Ng Wei Bo
Faculty of Dentistry, National University of Singapore

Deciduous teeth record development from mid-gestation and mark birth with a neonatal line, but straight transects and spot analyses cannot place elemental signals in developmental time [1,2]. We mapped Ca, Sr and Zn by synchrotron XFM at 1-2 μm in deciduous teeth from five children (three with atopic dermatitis, two without), registered the maps to polarised-light images, and sampled profiles along individual enamel rods anchored to each rod's neonatal line, using approximate daily secretion rates (~3-5 μm/day) [3]. Compared with rod-anchored profiles, a straight transect compressed the time axis by 10–50%, misdating signals by up to 2.5 weeks within a month of birth, and distorted Zn/Ca. Tracing the dentine-enamel junction to the dentine horn extended the incisor record to ~14 gestational weeks. Enamel Sr/Ca fell after birth in every child (−6% to −23%) while Ca was unchanged. Neonatal-line signatures differed between children (Zn or Sr enrichment, or a mineral-density dip), and simulated 35 μm spot sampling lost 42–85% of these contrasts. Accentuated lines in polarised light reflected porosity rather than elemental change. One child showed a candidate line about five weeks after a recorded infection. Birth-anchored XFM yields individual prenatal-to-postnatal elemental timelines; larger cohorts are needed to test associations with atopic dermatitis.

Reference(s):

1. Dean MC, Spiers KM, Garrevoet J, Le Cabec A. Synchrotron X-ray fluorescence mapping of Ca, Sr and Zn at the neonatal line in human deciduous teeth reflects changing perinatal physiology. Archives of oral biology. 2019 Aug 1;104:90-102.
2. Müller W, Nava A, Evans D, Rossi PF, Alt KW, Bondioli L. Enamel mineralization and compositional time-resolution in human teeth evaluated via histologically-defined LA-ICPMS profiles. Geochimica et Cosmochimica Acta. 2019 Jun 15;255:105-26.
3. Birch PD, Dean PD. A method of calculating human deciduous crown formation times and of estimating the chronological ages of stressful events occurring during deciduous enamel formation. Journal of forensic and legal medicine. 2014 Feb 1;22:127-44.

UM26-ABS-P12

Zone-specific trace element behavior in natural enamel caries

Tan Guang-Rong
Faculty of Dentistry, National University of Singapore

Tooth decay (caries) is the world's most common oral disease.[1] It begins in enamel through repeated cycles of demineralization, when acid dissolves the mineral, and remineralization, when saliva partly rebuilds it, creating distinct zones.[2] Trace elements in and around enamel make the mineral harder or easier to dissolve,[3–5] but their distribution across natural lesion zones remains largely unexamined. Because zones differ in porosity, crystal surface and organic content,[2,6,7] we proposed that, over these cycles, each element is lost or kept according to its binding strength and the binding sites and access each zone offers.[5,8] Using a synchrotron X-ray fluorescence microscope,[9] we mapped calcium and five trace elements at 1-µm steps across a natural lesion, comparing each point with apparently sound enamel at equal depth. The surface layer held less zinc and copper than the reference. The lesion body lost ~10% of its calcium and two-thirds of its strontium, yet held 9× the zinc and 18× the copper of the reference, relative to calcium. In the dark and translucent zones, zinc overtook copper, and bromine was trapped in the dark zone. These results suggest binding strength governs retention in the lesion body, whereas access and trapping govern the advancing front.

Reference(s):

1. GBD 2023 Oral Disorders Collaborators. Global and regional progress towards reduced burden of oral conditions between 2019 and 2023: a systematic analysis for the Global Burden of Disease Study 2023. Lancet Public Health. 2026;11(9):e630–e641. https://doi.org/10.1016/S2468-2667(26)00143-X
2. Robinson C, Shore RC, Brookes SJ, Strafford S, Wood SR, Kirkham J. The chemistry of enamel caries. Crit Rev Oral Biol Med. 2000;11(4):481–495. https://doi.org/10.1177/10454411000110040601
3. Featherstone JDB, Shields CP, Khademazad B, Oldershaw MD. Acid reactivity of carbonated apatites with strontium and fluoride substitutions. J Dent Res. 1983;62(10):1049–1053. https://doi.org/10.1177/00220345830620100801
4. Mohammed NR, Lynch RJM, Anderson P. Inhibitory effects of zinc ions on enamel demineralisation kinetics in vitro. Caries Res. 2015;49(6):600–605. https://doi.org/10.1159/000441014
5. Brookes SJ, Shore RC, Robinson C, Wood SR, Kirkham J. Copper ions inhibit the demineralisation of human enamel. Arch Oral Biol. 2003;48(1):25–30. https://doi.org/10.1016/S0003-9969(02)00162-0
6. Shellis RP, Hallsworth AS, Kirkham J, Robinson C. Organic material and the optical properties of the dark zone in caries lesions of enamel. Eur J Oral Sci. 2002;110(5):392–395. https://doi.org/10.1034/j.1600-0722.2002.21337.x
7. Palamara J, Phakey PP, Rachinger WA, Orams HJ. Ultrastructure of the intact surface zone of white spot and brown spot carious lesions in human enamel. J Oral Pathol. 1986;15(1):28–35. https://doi.org/10.1111/j.1600-0714.1986.tb00560.x
8. Smičiklas I, Onjia A, Marković J, Raičević S. Comparison of hydroxyapatite sorption properties towards cadmium, lead, zinc and strontium ions. Mater Sci Forum. 2005;494:405–410. https://doi.org/10.4028/www.scientific.net/MSF.494.405
9. Howard DL, de Jonge MD, Afshar N, Ryan CG, Kirkham R, Reinhardt J, et al. The XFM beamline at the Australian Synchrotron. J Synchrotron Radiat. 2020;27:1447–1458. https://doi.org/10.1107/S1600577520010152

UM26-ABS-P13

Progress on Decoding Hair physicochemical characterization

Husen Kang
Procter & Gamble International Operations SA Singapore

Hair quality depends on its hierarchical structure, particularly the α-keratin framework and the lipid-rich cell membrane complex (CMC). Both are altered by aging and cumulative damage, yet the underlying multi-scale mechanisms remain poorly understood.

We propose a multi-modal analytical approach to establish fundamental structure–chemistry relationships in human hair integrating SAXS/WAXS and MicroCT. Together, these data aim to connect molecular-level changes with hair strength and appearance. This will provide a mechanistic understanding of fundamental hair problems to guide the design of targeted solutions. These structure–chemistry links could also enable simpler, lab-based spectroscopic methods for future routine analysis.

Reference(s):

1. M. Kakizawa et al., Small-angle X-ray diffraction structural analysis of human hairs of different shapes and effect of straight perming, *JCSC*, 34(2), 102–107 (2010).
2. Y. Kajiura et al., Structural analysis of human hair single fibres by scanning microbeam SAXS, *J. Struct. Biol.*, 155(3), 438–444 (2006).
3. C. V. D. Berg et al., Quantifying whole human hair scalp fibres of varying curl: A micro-computed tomographic study, *J. Microsc.*, 297(2), 227–251 (2025).
4. H. A. Bechtel et al., Synchrotron infrared nano-spectroscopy and -imaging, *Surf. Sci. Rep.*, 75(3), 100493 (2020).

UM26-ABS-P14

Unveiling the intrinsic mechanics of silicate hydrogels in cementitious materials

Liu Chen
National University of Singapore

Silicate hydrogels are the main binding phases that give cement-based materials their strength and durability. This study will investigate how calcium, sodium and magnesium ions control their nanoscale structure and mechanical behaviour. Using synchrotron X-ray scattering with high pressure, we will track structural changes in real time across multiple length scales. The results will identify the key structural features governing stiffness, deformation and failure. By linking chemical composition, internal structure and mechanical performance, this research will provide practical guidance for designing more robust, durable and lower-carbon cementitious materials.

UM26-ABS-P15

Synchrotron Radiation Techniques for Investigating the Oxygen Evolution Reaction

Cui Wen
Department of Materials Science and Engineering, College of Design and Engineering,
National University of Singapore

Understanding the oxygen evolution reaction (OER) requires resolving how local coordination and electronic structure govern catalytic pathways and durability. This poster summarizes recent studies from our group that demonstrate the complementary roles of synchrotron techniques in OER research. Hard X-ray absorption spectroscopy, including XANES and EXAFS, probes metal oxidation states, coordination environments, and structural reconstruction, while soft X-ray absorption spectroscopy reveals metal–oxygen hybridization and oxygen-derived electronic states. Resonant inelastic X-ray scattering and X-ray magnetic circular dichroism further provide insights into electronic excitations and spin polarization. Representative studies address light-triggered oxygen redox at cobalt oxyhydroxide edges, electron-transfer processes underlying step-resolved OER kinetics, facet-selected oxygen-deficient ruthenium oxide for acidic oxygen evolution, spin-conserved radical oxygen coupling, and sequential electronic reconstruction for durable oxygen redox. By integrating synchrotron measurements with electrochemical kinetics, isotope-labeling experiments, vibrational spectroscopy, and theoretical calculations, these studies connect evolving catalyst structures with reaction mechanisms and device performance. Together, they illustrate how complementary synchrotron probes advance the identification of active configurations and guide the design of efficient, durable electrocatalysts for water electrolysis.

Reference(s):

1. *Nature* 2022, 611, 702–708.
2. *Nat. Sustain.* 2026, DOI:10.1038/s41893-026-01940-6
3. *Nat. Commun.* 2026, 17, 7417
4. *Nat. Commun.* 2026, 17, 7377.
5. *Nat. Commun.* 2026, 17, 10179.
6. *Nat. Commun.* 2026, 17, 10747.
7. *Adv. Energy Mater.* 2026,16, e06195.

Acknowledgements

The National Synchrotron Programme (NSP) would like to thank the following for contributing to this meeting –

1. Beamline Scientists, Users and Staff of the Singapore Synchrotron Light Source (SSLS);
2. Principal Investigators and Project Team Members of the Singapore-International Synchrotron Access Programme (SG-ISAP).

The National Synchrotron Programme (NSP) is supported by the National Research Foundation, Singapore.

© 2024 National Synchrotron Programme. All Rights Reserved.